Board 33: Work in Progress: Active Learning of Kinetics and Reactor Design Through a Jupyter Notebook

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1. Introduction

Kinetics and Reactor Design is one of the core courses in chemical engineering undergraduate education. This course is offered in the junior or senior year. The reaction engineering course has technical prerequisite courses. Moreover, the course is considered one of the first courses in which students learn core chemical engineering knowledge that requires formulating a mathematical model, solving it numerically using a computer software, analyzing the results, and finally being able to make an engineering judgment.

Till today, most engineering knowledge in classrooms (e.g. reactor design course) is communicated via textbooks and scientific articles using hardcopies, or softcopies as PDF files. When students are dealing with engineering problems that require mathematical computing, they will have access to theories with governing model equations in a text format. Depending on the complexity of the equations, the right numerical solver is applied to solve the numerical problem. These numerical solvers are supported with tutorials to explain how to use them and not the problem at hand. Sometimes, the program code is provided and most of the time not. To reproduce this knowledge and use it, an effort is needed to put all this fragmented knowledge together and re-establish a working model code. These working models are then used to teach students in an interactive environment and allow them finally to make engineering judgments. Therefore learning is mainly carried out in silos, and students have to put extra effort to connect these topics altogether and deepen their learning. The other common gap associated with traditional classrooms is that students' learning experience is often not connected to real-life challenges. Students feel that engineering courses are similar to mathematics because most of the provided problems are abstract. These problems don't teach students how to implement their engineering knowledge and sense to take the right decision in real-life situations or problems.

This research has two main aims. First, it aims to deepen the students' learning experience and avoid the silo learning approach in traditional classrooms. It explores active learning through the use of Jupyter notebook as an educational tool. Thanks to the advancement in the digital era to have mediums such as Python (open-source programming language) and Jupyter (Integrated development environment - IDE). Jupyter is a combination of open-source programming languages: Julia (Ju), Python, (Py), and R [1]. Although Jupyter notebooks are heavily used in machine learning and data science, some explored their power in modeling and teaching other fields of study [2]. Jupyter is an interactive web tool that can accommodate different programming code types, computational output, markdown text, and LaTex in a notebook form. It also allows adding figures and videos around the used code which is another interactive key feature. These features make Jupyter notebook unique with significant potential as a teaching medium. Python is easy to learn and fast to develop numerical solver. The available libraries in Python serve as a plus in academic research. Libraries like Numpy, Scipy, and Matplotlib have rich user interface experiences. Furthermore, the Python programming community is active and one of the largest communities available online. Google Colab supports Python and Jupyter notebook. Colab is a powerful online notebook where students can write and execute code on the cloud. There are many available resources to learn and know more about Jupyter notebook, Python, and Colab that are beyond the scope of this work.

The second aim of this research is to allow the students to foresee the link between what they learn and the impact on a real-life challenge. This will help them to develop a better sense of engineering judgment. In this research, the challenge of capturing CO_2 is taken as an example of a global environmental problem that can be solved with the use of a chemical reactor. Students will learn the core kinetics and reactor design fundamentals by designing a chemical reactor that can capture CO_2. In the future, other challenges that would require reactor design can be explored and applied instead of CO_2 capture as part of the reaction engineering course.

This research is still a work-in-progress and carried out in the following stages:

- First, the Jupyter notebook was developed and made available in a tutorial-like format. The first section introduces the main features of Jupyter notebook and the format of the tutorial. External links were provided where the students can learn and explore different applications of such open-source tools. Following that, a detailed background on the CO_2 emissions challenge was provided where students will get the motivation and a sense of responsibility towards their planet. CO_2 capture was suggested as one of the potential solutions to reach net zero emission targets. Based on the course requirements, the notebook explains the reactor design mathematical modeling and the associated fundamental kinetics for CO_2 capture. As explained earlier, Jupyter notebook allows writing Python code with the text. So, the numerical solution is present along with the theory and students can further investigate the reactor model and perform their own sensitivity studies.

- In the second stage, the tutorial is offered to 5 chemical engineering undergraduate students researching a similar topic, but they did not have a background in reactor modeling and had a basic knowledge of Python. Anecdotal feedback has been gathered from the students on a one-to-one basis. Students could not utilize the tutorial on their own and needed some support in the beginning, to better navigate and understand how this tutorial and code work, as this approach was new to them. All students successfully demonstrated their ability to utilize this tool and do some parametric studies using it. Overall, they gave positive feedback and wanted to have a similar approach in the future. However, they all recommended starting with a simpler case first to understand the learning method, then moving forward to a more advanced tutorial as the one offered to them.

- The final stage is to introduce this intervention in the classroom for all students who are taking the Kinetics and Reactor Design. A structured assessment needs to be established to assess the students' learning experience. At the moment, the intention for the structured assessment is to provide the same questionnaire (in the form of reflection questions) to two different classes. The first class will be implementing Jupyter notebook as a tool in the assignments and course project along with in-class tutorials on how to use the notebook combined with Python, while the second class will be applying the traditional approach. This stage is not yet done as this is still a work in progress. Nevertheless, the plan is to introduce this new approach next year when the kinetics and reactor design course is offered.

Presenting this research at the 2023 ASEE annual conference, while it is still at the progress stage, enables us to interact with other instructors who have done something similar to share experiences and to develop our structured assessment for next year’s intervention. In principle, the proposed intervention can be implemented in other engineering courses that have a similar

teaching challenge and require a computational approach. Following the classroom experience, we will share our findings and the students' feedback at the 2024 ASEE conference. So, instructors from different fields of study can even apply this valuable tool in their classrooms.

To provide an idea of what has been developed, two sections are given below to explain the tutorial in Jupyter notebook and the theory that needs to be learned along with the CO_2 capture challenge.

2. Example of application, theory, and fundamental students need to learn

2.1.Motivation and application challenge

Responding to global warming is a responsibility of our time to avoid the foreseen effects like droughts, heavy precipitation, heat waves, and rising sea levels [3]. Many countries are currently committed to addressing this challenge and meeting the UN's Sustainable Development Goals [4]. CO_2 is a major contributor to global warming. Indeed, CO_2 capture is a very promising solution to reduce CO_2 emissions and the global warming effect. There are different CO_2-capturing technologies available today. Amine absorption is widely applied in the industry due to its high maturity. Amines absorb CO_2 physically and chemically. The former is due to the solubility of CO_2 in amines while the latter is due to the chemical reaction between CO_2 and amines in the liquid phase [5]. MEA (monoethanolamine) is the most used CO_2 absorbent due to its low cost, high performance at low pressure, and fast reaction rate with CO_2 [6]. Although CO_2 absorption is a mature technology with commercial applications, implementing it at a large scale requires reducing the associated costs significantly and being able to accommodate different types of gas emission sources. Thus, there is still an urgent need to study this technology and improve it.

Microreactors are an emerging technology in chemical reaction engineering [7]. The high surface area to volume ratio is an important characteristic of the microreactor design. It reduces the mass and heat transfer resistances resulting in superior mass and heat transfer rates, compared to larger reactors [8]. Microreactors easily and precisely control the flow and temperature conditions which results in a high potential for process intensification for several engineering applications. Microreactor technology is being explored for CO_2 post-combustion capture (PCC) because of the high mass transfer and controlled temperature operation [9], [10]. Ganapathy et al. reported substantial levels of process intensification achieved by microreactors for CO_2 absorption [11].

Gas-liquid flow in a microchannel generates different flow regimes depending on the flow rates used. The Taylor flow is characterized by an alternating arrangement of elongated cylindrical gas bubbles and liquid slugs as shown in Figure 1. Taylor flow offers high mass transfer rates and low axial dispersion due to the vortices inside the liquid slugs [12], [13]. The flow regime is essential in the reactor design and modeling as it determines the gas-liquid interfacial area, mixing phenomena, pressure drop, and gas and liquid hold-up. In this work, the Talor flow was maintained because higher CO_2 absorption efficiencies can be achieved.

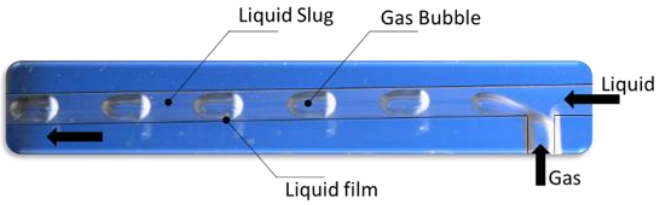

Figure 1: Hydrodynamics of Taylor flow

2.2.Fundamentals of reaction

The reaction mechanism is important to understand the reaction kinetics in the reactor model. In chemical absorption, CO_2 reacts with amines in the liquid phase only. The reaction between CO_2 and amines produces carbamate (bicarbonates) according to two mechanisms: Zwitterion and Termolecular [5]. In this study, the zwitterion mechanism was applied to describe the CO_2 absorption kinetics. The carbamate ($MEACOO^-$) and protonated base ($MEAH^+$) are the final products of the overall reaction (R-1).

$$CO_2 + 2MEA \overset{k_3}{\leftrightarrow} MEACOO^- + MEAH^+ \qquad (R-1)$$

First, the zwitterion is formed ($MEAH^+COO^-$) as shown in reaction 2 (R-2). Then, it undergoes deprotonation by a base B (R-3). The main contribution to the deprotonation of the zwitterion comes from MEA (amine) since the deprotonation ability depends on the concentration of the base B (R-4). The other species like OH^-, HCO^{3-}, and H_2O have negligible concentrations and don't contribute to deprotonation [14]. Thus, MEA will act as the base B in reaction 3 (R-3).

$$CO_2 + MEA \overset{k_1}{\leftrightarrow} MEAH^+COO^- \qquad (R-2)$$

$$MEAH^+COO^- + B \overset{k_2}{\leftrightarrow} MEACOO^- + BH^+ \qquad (R-3)$$

$$MEAH^+COO^- + MEA \overset{k_2}{\leftrightarrow} MEACOO^- + MEAH^+ \qquad (R-4)$$

If the deprotonation of zwitterions is faster than their formation, the zwitterion formation will be the rate-determining step (R-2). So, the reaction rate implemented in this work will be as follows:

$$r_{CO_2} = k_1[MEA][CO_2]$$

Most kinetic approaches in the literature follow the simple bimolecular kinetic law shown above [15]. The explained bimolecular kinetic approach will be applied in the following reactor model.

Finally, a one-dimension ideal plug flow reactor model is being developed at isothermal conditions. The main assumptions are listed, below:

(1) Pressure drop is neglected to simplify the given demonstration.
(2) Taylor flow regime is maintained throughout the entire work.
(3) The reaction is assumed to take place in the liquid phase.
(4) Gas bubble length, superficial velocities, and hold-ups are estimated at the inlet conditions of the microreactor.

(5) Liquid slug length is assumed to remain the same across the channel.
(6) The mass transfer takes place in the available gas-liquid interface where only CO_2 is exchanged between the two phases.

2.3.Fundamental of mathematical modeling

The reactor design equations are shown below as a result of the mass balance on the gas and liquid sides, respectively.

$$\frac{dC_{CO_{2,G}}}{dz} = -\frac{1}{u_G} j_{CO_2} \qquad (E-1)$$

$$\frac{dC_{i,L}}{dz} = \frac{1}{u_L}(j_i + r_i \varepsilon_L) \qquad (E-2)$$

Where i in equation 2 (E-2) refers to the the following components: CO_2, MEA, MEAH, MEACOO. Table 1 shows the supporting correlations needed to model the CO_2 chemical absorption by MEA (primary amine) in a microreactor.

Table 1: Reactor model equations and supporting correlations

Referece	E - #	Equation Type	Equation	Linked section
	E - 3	Liquid holdup	$\varepsilon_L = 1 - \varepsilon_G$	
[16]	E - 4	Gas holdup	$\varepsilon_G = 0.833 \times \beta_G$	
[16]	E - 5	Dynamic gas holdup	$\beta_G = \frac{u_G}{u_G + u_L}$	
	E - 6	Gas superficial velocity	$u_G = \frac{q_G}{A}$	
	E - 7	Liquid superficial velocity	$u_L = \frac{q_L}{A}$	Taylor flow hydrodynamics
	E - 8	Two-phase superficial velocity	$u_{TP} = u_G + u_L$	
	E - 9	Bubble superficial velocity	$u_B = u_{TP}$	
[17]	E-10	Bubble length	$L_B = \left(1 + 0.57\frac{u_G}{u_L}\right) d_h$	
[17]	E-11	Slug length	$L_S = \frac{\left(1 + 0.57\frac{u_G}{u_L}\right) d_h (1 - \beta_G)}{\beta_G}$	
[15]	E-12	Main reaction rate expression	$r_{CO_2} = k_1 C_{MEA} C_{CO_2}$	Reactor kinetics
[18]	E-13	Rate constant	$k1 = 1.09 \times 10^9 \exp(-\frac{2671.4}{T})$	
	E-14	Mass transfer correlation	$j_{CO_2} = k_L a \left(C_{CO_{2,G}} - C_{CO_{2,L}}\right)$	Mass transfer
[19]	E-15	Volumetric mass transfer coefficient	$K_L a = \frac{0.111(u_G + u_L)^{1.19}}{\left((1 - \varepsilon_G) L_{UC}\right)^{0.57}}$	

3. Example of the tutorial structure

The outline structure of the tutorial on Jupyter notebook is explained in Figure 2. The input section includes importing Python libraries and defining the components, reactor dimensions,

and inlet conditions. Then, kinetics, hydrodynamics, and mass transfer follow where different correlations are implemented to find the reaction-rate constant, hydrodynamics parameters, and mass transfer coefficient. The last section of the tutorial includes the ODE (ordinary differential equation) solver and visualization where the students can observe the effect of different parameters on the reactor performance and further improve their understanding of the microreactor model.

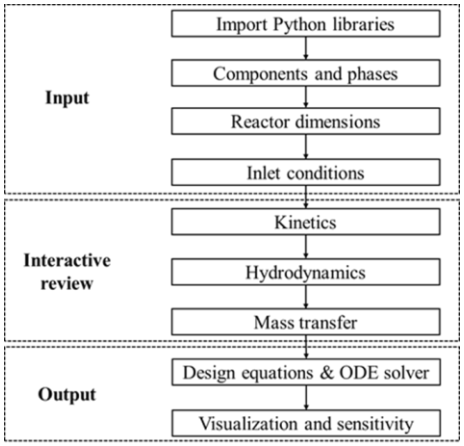

Figure 2: Tutorial outline

The interactive review section includes the correlations, code, and results of the different correlations. In the future, these correlations can be coded in Jupyter using Python to directly have a sense of their variations and applicability. The gas hold-up was selected as a small demonstration where three different correlations from literature are coded and executed to get the bar chart as shown in Figure 3.

1. Markdown cell

Index	Correlation	Description
Ie1	$\epsilon_G = \beta_G$	Homogeneous model
Ie2	$\epsilon_G = 0.833\beta_G$	Armand correlation
Ie3	$\epsilon_G = \frac{0.03\beta_G^{0.5}}{1-0.97\beta_G^{0.5}}$	Non-linear correlation
Ie4	$\epsilon_G = \frac{L_b}{L_b+L_s}$	Experimental method

2. Python code

```
Ie0 = 0 # user-inputted gas-holdup

Ie1 = beta_G
Ie2 = 0.833*beta_G
Ie3 = 0.03*beta_G**0.5/(1-0.97*beta_G**0.5)
Ie4 = Lb/(Lb+Ls)

df_e = pd.DataFrame({'eps G':['Ie0','Ie1','Ie2','Ie3','Ie4'],\
                     'NA': [Ie0,Ie1,Ie2,Ie3,Ie4]})
ax_e = df_e.plot.barh(x='eps G',figsize=(5,5), legend =False)
plt.grid(alpha=0.5)
plt.xlim(0,1)

eps_G = Ie2 # gas-holdup used in the simulation code
eps_L = 1- eps_G # liquid-holdup used in the simulation code
```

3. Results

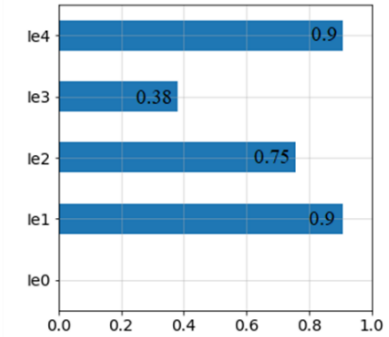

Figure 3: Intercative review demonstration on gas-holdup parameter

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